

# **Ba<sub>3</sub>BiPbREO(BO<sub>3</sub>)<sub>4</sub> (RE =Pr, Nd, Gd, Dy): Two-Dimensional Rare-Earth Antiferromagnets with Geometrically-Perfect Triangular Lattice Directed by Triangular BO<sub>3</sub> Unit**

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<i>RE</i>		<b>Pr</b>	<b>Nd</b>	<b>Gd</b>	<b>Dy</b>
<i>a</i> (Å)		5.3971(1)	5.4040(1)	5.4289(1)	5.4188(1)
<i>c</i> (Å)		26.9444(3)	26.8712(3)	26.3741(3)	26.2776(3)
<i>V</i> (Å <sup>3</sup> )		679.71(1)	679.60(1)	673.17(1)	668.22(1)
	<i>x</i>	0	0	0	0
<b>RE</b>	<i>y</i>	0	0	0	0
	<i>z</i>	1/2	1/2	1/2	1/2
	<i>x</i>	0	0	0	0
<b>Bi</b>	<i>y</i>	1	1	1	1
	<i>z</i>	0.3301(1)	0.6686(1)	0.6667(1)	0.6663(1)
	<i>x</i>	0	0	0	0
<b>Pb</b>	<i>y</i>	1	1	1	1
	<i>z</i>	0.3301(1)	0.6686(1)	0.6667(1)	0.6663(1)
	<i>x</i>	2/3	2/3	2/3	2/3
<b>Ba1</b>	<i>y</i>	1/3	1/3	1/3	1/3
	<i>z</i>	0.4090(1)	0.5900(1)	0.5880(1)	0.5869(1)
	<i>x</i>	2/3	2/3	2/3	2/3
<b>Ba2</b>	<i>y</i>	1/3	1/3	1/3	1/3
	<i>z</i>	1/4	3/4	3/4	3/4
	<i>x</i>	1/3	1/3	1/3	1/3
<b>B1</b>	<i>y</i>	2/3	2/3	2/3	2/3
	<i>z</i>	0.447(2)	0.5495(16)	0.5505(12)	0.5511(8)
	<i>x</i>	1/3	1/3	1/3	1/3
<b>B2</b>	<i>y</i>	2/3	2/3	2/3	2/3
	<i>z</i>	0.3195(15)	0.6803(14)	0.6758(17)	0.6743(1)
	<i>x</i>	0	0	0	0
<b>O1</b>	<i>y</i>	1	1	1	1
	<i>z</i>	1/4	3/4	3/4	3/4

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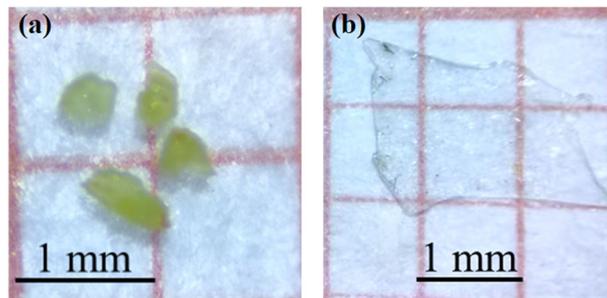
	<i>x</i>	0.4702(9)	0.4772(9)	0.4791(9)	0.4773(7)
<b>O2</b>	<i>y</i>	0.5298(9)	0.5228(9)	0.5209(9)	0.5227(7)
	<i>z</i>	0.3326(6)	0.6646(6)	0.6702(6)	0.6712(6)
	<i>x</i>	0.598(2)	0.198(2)	0.194(2)	0.194(2)
<b>O3</b>	<i>y</i>	0.869(5)	0.396(2)	0.388(2)	0.389(2)
	<i>z</i>	0.4494(5)	0.5492(5)	0.5529(4)	0.5512(3)
	$\chi^2$	8.60	9.54	4.65	8.45
	$R_{wp}$	0.117	0.127	0.129	0.106

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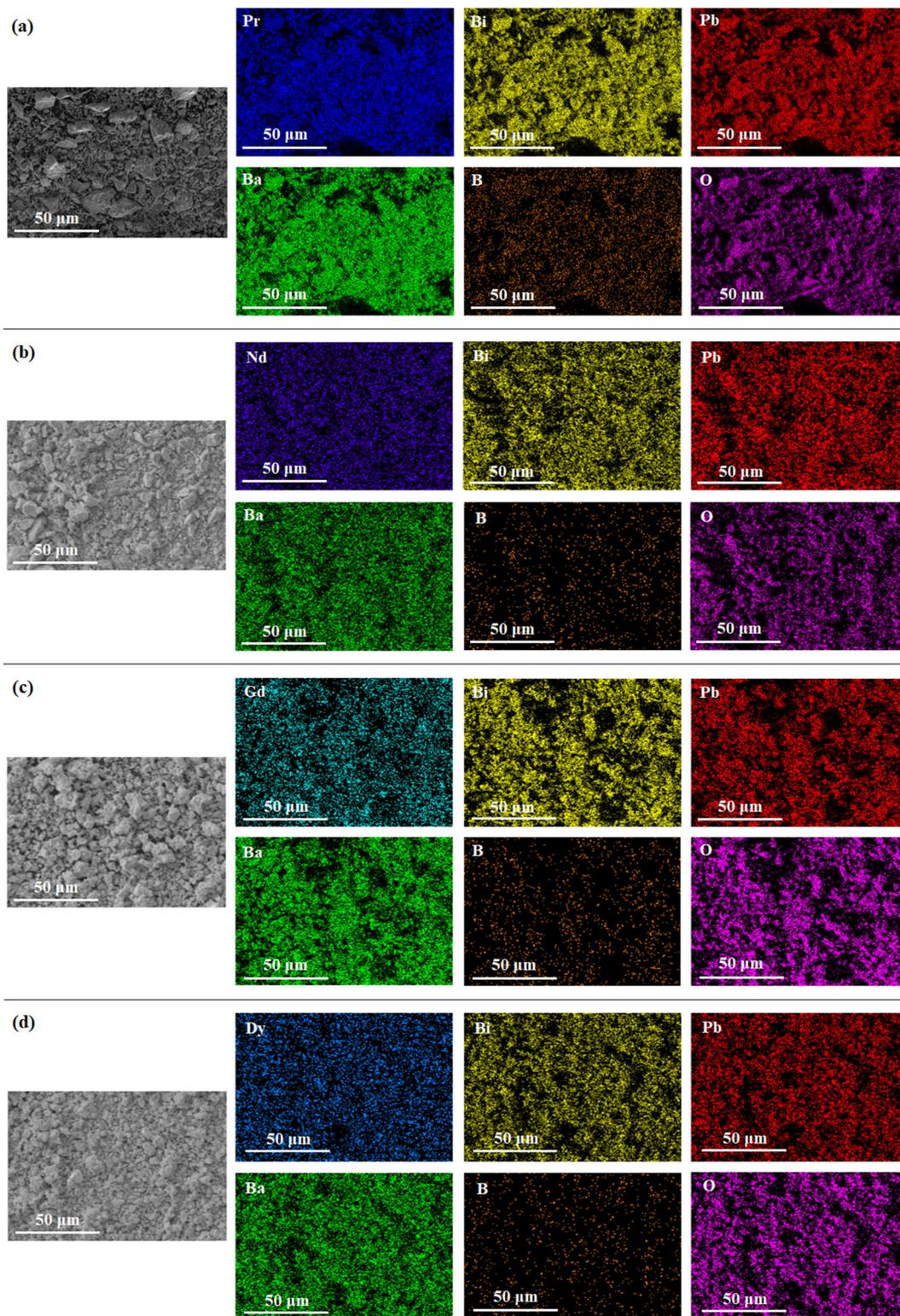
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Distances	Length/Å			
	Pr	Nd	Gd	Dy
RE–O	2.303(19)	2.277(11)	2.265(12)	2.267(8)
RE–RE <sub>intra</sub>	5.394(2)	5.404(1)	5.439(1)	5.419(1)
RE–RE <sub>inter</sub>	13.470(4)	13.436(1)	13.192(1)	13.139(1)
B–O	1.355(19)	1.267(9)	1.371(12)	1.304(8)
	1.360(20)	1.411(13)	1.386(15)	1.354(5)

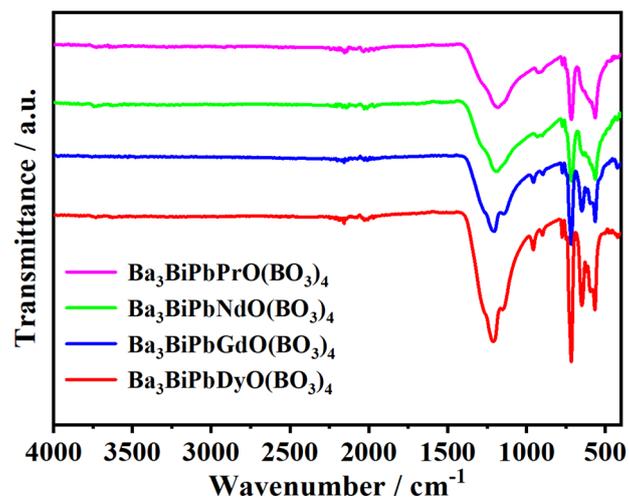
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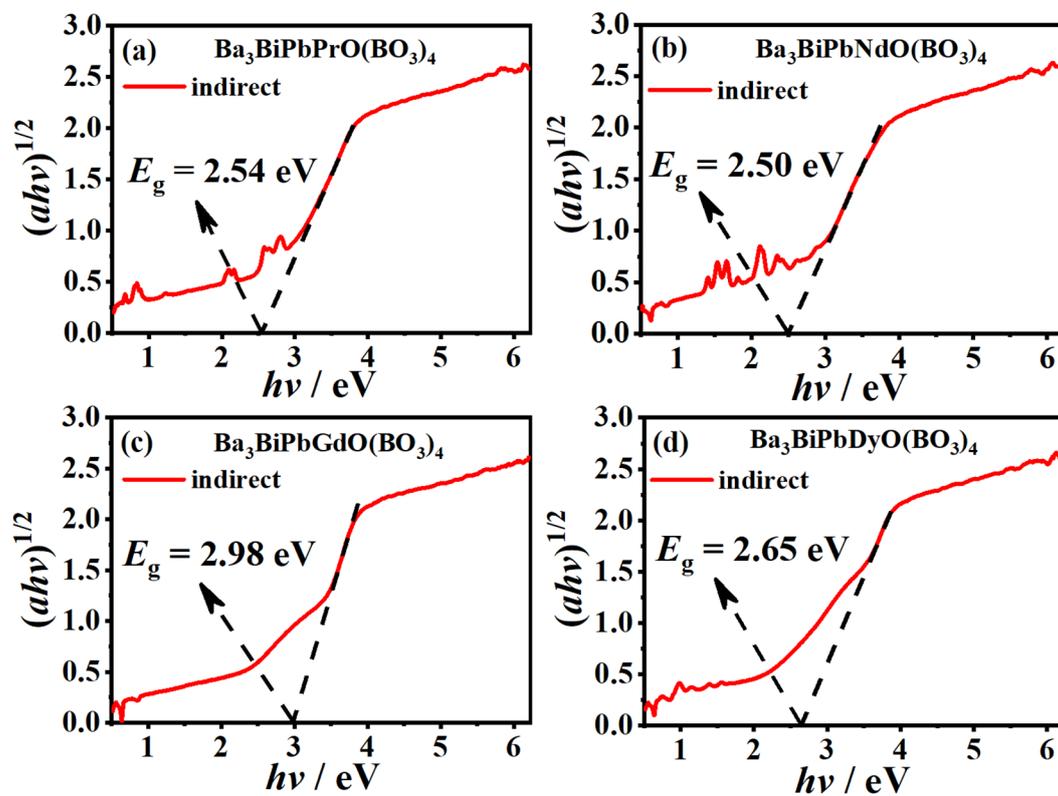
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